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Mechanical Properties of Multiwalled Carbon Nanotubes Toughened Quartz Nanocomposite  
Using Artificial Neural Network (ANN)

By

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### ABSTRACT

*Sequel to the experimental results acquisition using the established test procedures as outlined in the previous study on the manufacturing and mechanical characterization of multiwalled carbon nanotubes/quartz nanocomposite, the present research has been centred on the implementation and evaluation of an artificial intelligence model for the characterization of the multiwalled carbon nanotubes (MWNTs) reinforced quartz ceramic nanocomposite. A multi input and multi output Artificial Neural Network (ANN) model was developed using the Levenberg Marquardt Back Propagation (LMBP) algorithm to predict the mechanical properties of the MWNTs/quartz nanocomposite bricks developed in the previous study. The predicted model was compared with the experimental test results in order to evaluate the power and the accuracy of the artificial intelligence model for the characterization of the entire series of the nanocomposite bricks developed. The developed model adequately predicts the mechanical properties; specifically tensile and compressive strengths of MWNTs/quartz nanocomposite with a coefficient of determination ( $R^2$ ) in excess of 0.92.*

### INTRODUCTION

#### *Artificial neural network (ANN)*

The artificial neural network (ANN) is a computer based programs inspired by the capacity of the human brain in processing information. An outstanding feature of the ANN is that, rather than relying upon mere computer programs, the intelligence system offers great computational power to model complicated nonlinear processes by repeated training of a set of data until the output gives an acceptable value that correlates with the expected target (Jain *et al.*, 1996). Generally, the artificial neural network technique is highly robust and gives a satisfactory degree of accuracy. Apart from this, ANNs are very helpful in predicting the properties of new materials prior embarking on experimental study.

As depicted in Figure 1.0, an artificial neuron is comprised of five main parts: inputs, weights, sum function, activation function and outputs (Nazari and Riahi, 2011, 2013). The neurons receive input signals that are then scaled by the associated weights. The effect of inputs and weights are then completely calculated by the sum function which then computes

the net input approaching the neuron (Günaydın and Do an, 2004). The weighted sums of the input component are evaluated by employing equation 1.0

$$(n )_j = \sum_{i=1}^n w_{i,j} x_i + b \tag{1.0}$$

Where  $(n )_j$  is the weighted sum of the jth neuron for the input received from the previous layer with n neurons,  $\sigma$  is the sum function,  $w_{i,j}$  is the weight between the jth neuron in the preceding layer,  $x_i$  and is the output of the ith neuron in the previous layer and b is a fixed value as internal addition.

Afterwards, the combinations of the inputs are sent to an activation function whose function is to process the input obtained from the sum function and determines the neuron output.

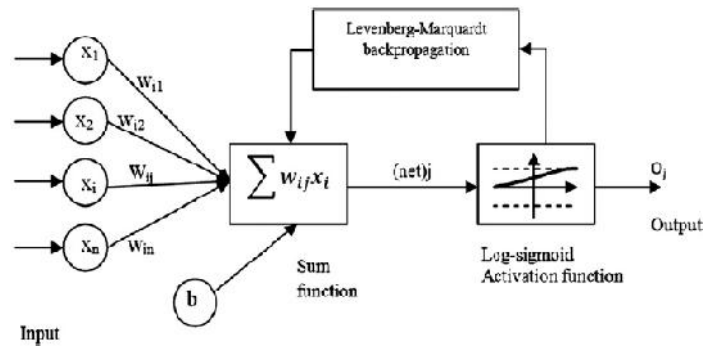


Figure 1.0: Architecture of artificial neural network (Nazari and Riahi, 2011, 2013)

At the same time, the performance accuracy of the selected ANN architecture can be estimated using various statistical parameters such as the mean square error (MSE), mean absolute error (MAE), normalized root mean square error (NSE) and mean absolute percentage error (MAPE) using equations 2 – 5 (Shabani *et al.*, 2012b):

$$M = \frac{1}{Q} \sum_{o=1}^Q \sum_{n=1}^{N_o} |d_n(m) - y_n(m)|^2 \tag{2}$$

$$M = \sum \left| \frac{x - y}{n} \right| \tag{3}$$

$$N = \sqrt{\frac{\sum(A - F)^2}{A^2}} \tag{4}$$

$$M = \left[ \frac{1}{N_o} \sum_{N=1}^{N_o} \left| \frac{A - F}{A} \right| \right] \times 100 \tag{5}$$

$N_o$  = the number of output.

Q = the number of training sets.

d = desired output.

y = Y -  $Y^1$  ; Y is the network output and  $Y^1$  is the mean of Y.

x = X -  $X^1$  ; X is the target output and  $X^1$  is the mean of X.

A = actual values.

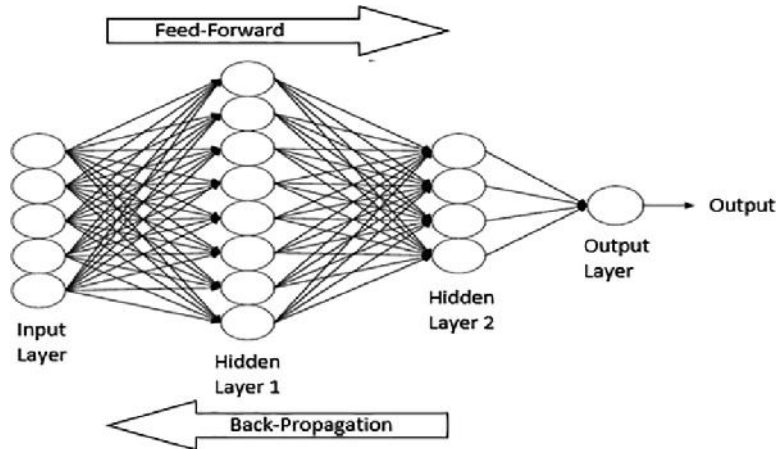
F = forecasted values.

**Back propagation ANN architecture and algorithm**

For many years, it has been widely established that the overall performance of an ANN is dependent on factors such as the topology of the ANN, the training algorithm as well as the choice of network parameters such as the transfer function, learning rate and momentum rate. Rumelhart *et al.* (1986); in their study, developed a learning algorithm called back-propagation, having embedded hidden units for perceptron networks, which is now the most widely used learning algorithms. A typical architecture of a multilayer perceptron neural network having an input layer, two hidden layers and an output layer is presented in Figure 2 (Nazari and Riahi, 2011, 2013). Generally, a sigmoid activation function; equation 6, is often utilized for the multilayer feed-forward model in order to compute the output of the  $j$ th neuron ( $\sigma_j$ ) (Hopfield, 1982). The sigmoid nonlinearity function gives output in (0,1) and it activates in every layer with the exception of the input layer (Liu and Liu, 2002).

$$O_j = f(n_j) = \frac{1}{1 + e^{-\alpha(n_j)}} \quad 6$$

Where  $\alpha$  is a constant used to control the slope of the semi-linear region.



**Figure 2:** A typical architecture of multilayer perceptron neural network (Nazari and Riahi, 2011, 2013)

Furthermore, investigations so far (Nazari and Riahi, 2011, 2013; Shabani *et al.*, 2012a) have shown that out of the different training algorithms for back propagation such as, Gradient Descent with Adaptive Learning Rate (GDA), Levenberg-Marquardt (LM), Bayesian Regularization (BR), Scaled Conjugate Gradient (SCG), the Levenberg-Marquardt Back Propagation (LMBP) seems to be the first-choice and fastest available algorithm. The LMBP algorithm operates on a layer-by-layer basis by modifying the weight and bias values of the various layers of an ANN with the view to repeatedly minimize the error function until a stop criterion or specified minimum value is attained (Wilamowski and Yu, 2010). With the utilization of the LMBP training algorithm, the adaptation of the weights can be determined as follows:

$$w = [J^T J + \mu ]^{-1} J^T e \quad 7$$

Where J is the Jacobian matrix and  $\mu$  is the learning rate.

Hitherto, quite a number of models have been proposed to predict the mechanical properties of composite materials using artificial neural network viz. (Nwobi-Okoye and Ochieze, 2018; Tuntas and Dikici, 2016). Varol *et al.* (2018) employed the multilayered neural network (MLP) trained with back propagation algorithm to develop a neural network model for the prediction of the density and hardness values of SiC reinforced AA 2024 nanocomposites. The researchers observed a highly reliable performance of the prediction model with the density and hardness in the testing process exhibiting root mean square errors (RMSE) of 0.006% and 0.835% respectively.

By a comparative study, Nwobi-Okoye and Ochieze (2018) utilized both the response surface methodology (RSM) and artificial neural network (ANN) to independently develop prediction models for predicting the hardness value of aluminium alloy A356/cow horn particulate composites. They reported that the ANN exhibited better accuracy than the RSM in predicting the hardness values of the composites. Despite their proposition regarding the ANN model being a powerful tool for the prediction of the physical properties of traditionally prepared barium titanate ceramics, Al-Jabar *et al.* (2017) highlighted the limitation of the model as its constrained ability of predicting values within the range of the experimental study. Thus, they suggested an extension in the limits of the experimental parameters for future studies.

Finally, with an inclination towards creating an artificial intelligence model that can minimize rigorous experimental runs and supply useful instruction in the development of various composites and advanced materials, the artificial neural network has gained tremendous momentum amidst experts in the field of materials engineering. Up to now, from the studies reviewed, quite a number of investigators have revealed a satisfactory result by using the Levenberg-Marquardt Back Propagation (LMBP) algorithm in the characterization of various materials for instance; alloys and composites. Therefore, the ANN prediction model with LMBP training algorithm would be built and deployed in the current study to optimize and predict the mechanical properties of the developed MWNTs/quartz ceramic nanocomposite systems.

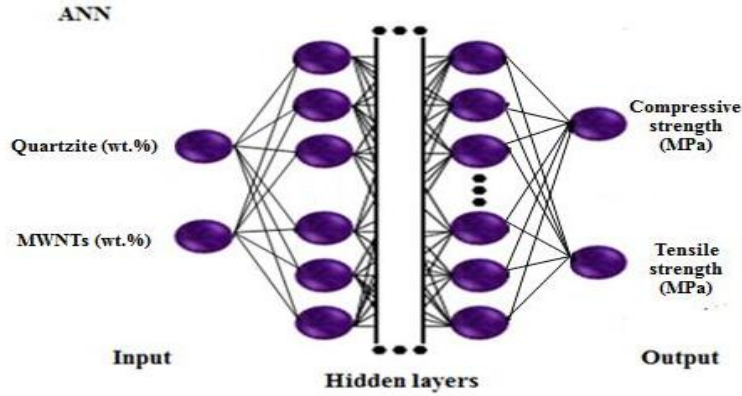
## THE ANN MODELING

A total of 11 data patterns; input and output, collected from all sample formulations were used in training the ANN. The overall data in the model was divided into three categories, consisting of training (80%), validation (10%) and testing (10%). It is also worth noting that both the input and output data were normalized within a range of 0 and 1 with the aids of equation 8, in order to ensure the proper execution of the sigmoid transfer function.

$$X_n = \frac{X - X_m}{X_m - X_m} \quad 8$$

Where  $X_n$  is the normalized value,  $X$  is the true value of the variable,  $X_m$  and  $X_m$  are the minimum and maximum values of the dataset respectively.

The network model in ANN was programmed by a supervised multilayer perceptron (MLP) trained with the back propagation (BP) algorithm from the neural network toolbox of MATLAB R2015a. For the ANN (Figure 3), MLP ANN containing two input parameters (Quartzite content and MWNTs content) and two output parameters (tensile strength and compressive strength) was developed and evaluated.



**Figure 3:** ANN model for characterizing the MWNTs/quartz nanocomposite

Due to the lack of standards for the determination of the required hidden layers and neurons, preliminary investigation revealed that two hidden layers gave the best performance value; minimum absolute error values for the training and testing data sets relative to one hidden layer. Thus, while investigating the optimum number of neurons required to build the neural network models, the number of hidden layers was fixed at two for the ANN model. Furthermore, after several iterations the best ANN topology was selected based on (i) the tan-sigmoid transfer function; equation 9 in both hidden layers, (ii) a linear transfer function; equation 10 in the output layer and (iii) best performance criteria; which is the function of goodness of fit of the different ANN topologies tested and based on the three statistical parameters; coefficient of determination ( $R^2$ ), root mean square error (RMSE) and mean absolute error (MAE), equations 11 and 12.

$$T \quad (n) = \frac{2}{(1 + \exp(-2n)) - 1} \quad 9$$

$$P \quad (n) = n \quad 10$$

$$R = \sqrt{\frac{\sum_{i=1}^N (y_p^i - y_t^i)^2}{N}} \quad 11$$

$$M = \frac{1}{N} \sum_{i=1}^N |y_p^i - y_t^i| \quad 12$$

Where  $y_p^i$  is the predicted value,  $y_t^i$  is the real value retrieved from the experimental data and  $N$  is the number of observations.

**Levenberg-Marquardt Back Propagation (LMBP) Algorithm**

In spite of consuming a relatively higher memory and processing resources than other algorithms, the LMBP has been adopted in the current study as the training algorithm due to its high efficiency and accuracy.

**Performance of the LMBP-ANN models**

In order to validate the performance of the LMBP ANN in characterizing the different grades of MWNTs reinforced quartz ceramic nanocomposites developed in the previous study (Tijjani *et al.*, 2018), various ANN topologies were deployed in training the network by adjusting the number of hidden neurons. Table 1 highlight the network performance for each of the ANN topology; hidden neuron configuration employed in developing the ANN model.

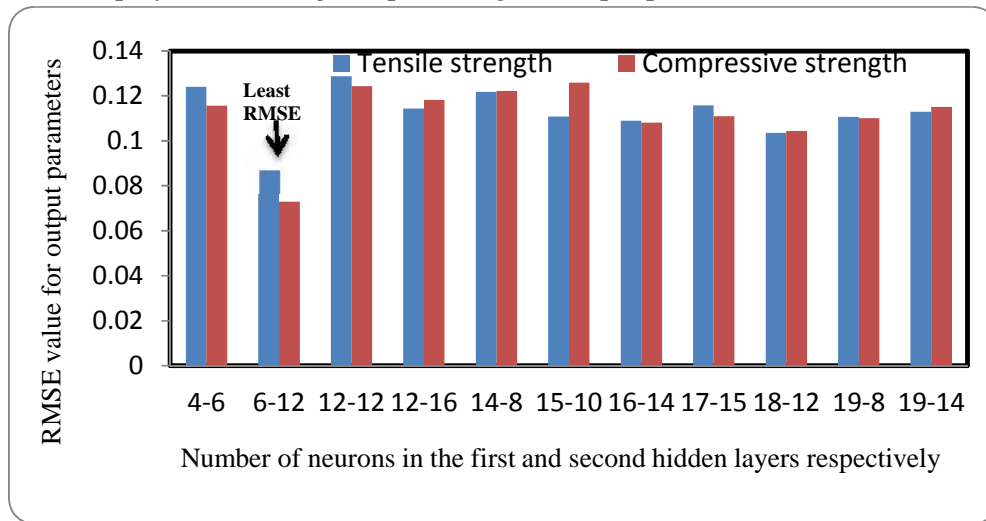
Eleven (11) different ANN topologies were tested by systematically varying the number of neurons in the hidden layers (between 4 and 20).

**Table 1: Variation of hidden neurons utilized in developing the ANN model**

Hidden neurons	Train			Validation			Test		
	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>	RMSE	MAE	R <sup>2</sup>	RMSE	MAE
4-6	0.9334	0.1674	0.1401	1.0000	0.1455	0.1455	1.0000	0.0146	0.0146
6-12*	0.9777	0.1011	0.0717	1.0000	0.0954	0.0954	1.0000	0.1992	0.1992
12-12	0.9314	0.1940	0.1416	1.0000	0.0741	0.0741	1.0000	0.0855	0.0855
12-16	0.9622	0.1477	0.1306	1.0000	0.2611	0.2611	1.0000	0.0508	0.0508
14-8	0.9314	0.1845	0.1280	1.0000	0.0858	0.0858	1.0000	0.1069	0.1069
15-10	0.9304	0.1748	0.1355	1.0000	0.1748	0.1748	1.0000	0.0214	0.0214
16-14	0.9492	0.1534	0.1265	1.0000	0.1103	0.1103	1.0000	0.1847	0.1847
17-15	0.9222	0.1617	0.1418	1.0000	0.0063	0.0063	1.0000	0.0053	0.0053
18-12	0.9509	0.1492	0.1158	1.0000	0.1028	0.1028	1.0000	0.0859	0.0859
19-8	0.9407	0.1439	0.1134	1.0000	0.1409	0.1409	1.0000	0.2483	0.2483
19-14	0.9359	0.1735	0.1503	1.0000	0.0244	0.0244	1.0000	0.1146	0.1146

\* Best model based on the training, validation and test data.

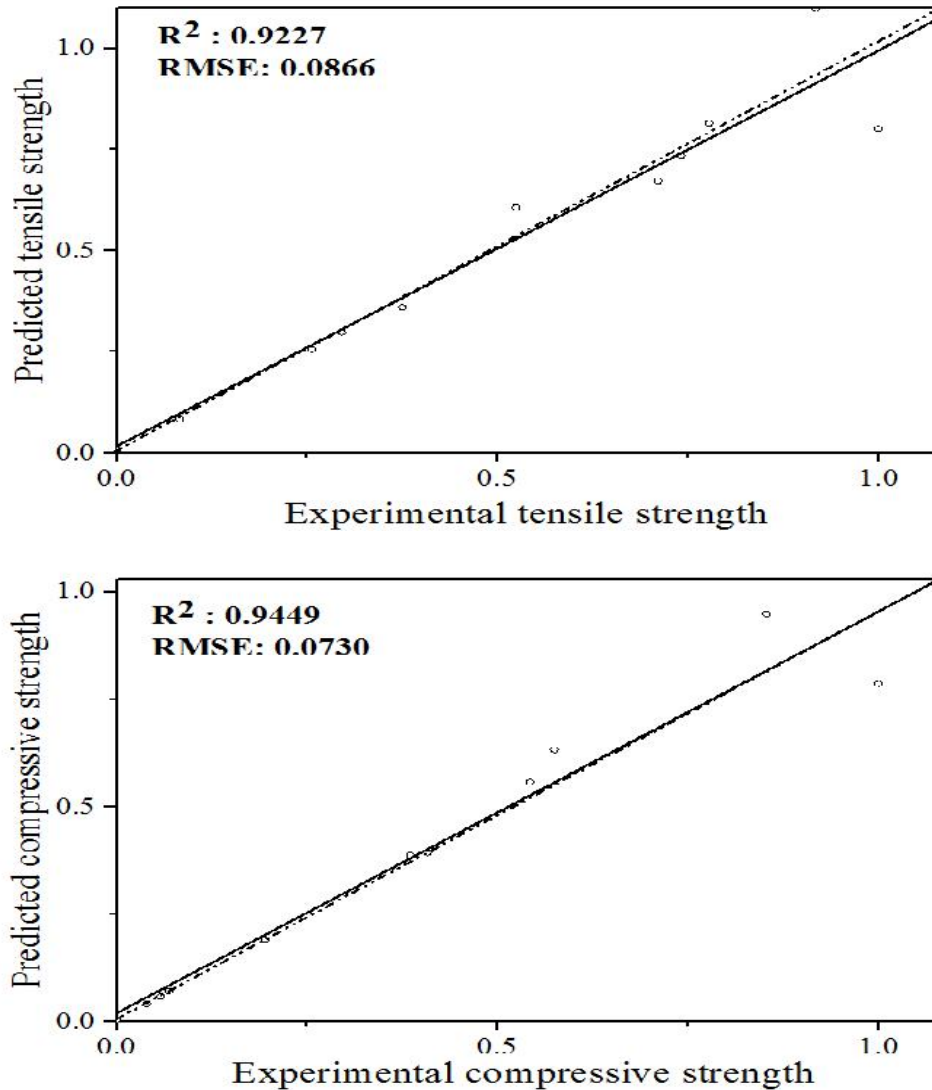
Using the RMSE values of the different ANN topologies tested, the performances of the ANN model in predicting the output parameters are graphed in Figure 4. From both the Table 1 and Figure 4, it is evident that the best hidden neuron configuration based on the highest coefficient of determination (R<sup>2</sup>), lowest training error (RMSE and MAE), and the least RMSE of the predicted output parameters, is 6-12 for the dataset trained in the model ANN. Hence, the 2-6-12-2 was selected as the preferred and the most accurate ANN architecture deployed in training and predicting the output parameters of the ANN.



**Figure 4:** The performance of the ANN in characterizing MWNTs/quartz nanocomposite in terms of RMSE value

As can be observed from Figures 5, the predicted values determined by using the optimum ANN topology in the model are close to the experimental results. Even though the deviation of some points is obvious; this may be attributed to limited experimental dataset

employed for training the ANN model. For the ANN model,  $R^2$  values  $> 0.92$  was obtained for the output parameters. As seen from the figures a good fit between the experimental values (the straight line) and the predicted values (the data points); the proposed ANN model has the ability to satisfactorily predict with a minimal error, the mechanical properties; tensile and compressive strengths of MWNTs/quartz nanocomposite having formulations within the range of those employed in the experimental process of the previous study by Tijjani *et al.* (2018).



**Figure 5:** Comparison between predicted and experimental results for the MWNTs/quartz nanocomposite

**CONCLUSION**

This study presents a supplementary approach to that of the experimental processes adopted by Tijjani *et al.* (2018), using intelligent computing model (LMBP ANN model). Thus, a means of accurately predicting the mechanical properties of the MWNTs/quartz

nanocomposite. The LMBP ANN model analysis in terms of the  $R^2$ , RMSE and MAE showed that the choice of the hidden layer size and number of hidden layer neurons are the two most sensitive parameters in efficiently training the overall dataset as well as achieving the desired predicted results. The accuracy and performance efficiency of the developed model; ANN was confirmed by the large coefficient of determinant ( $> 0.92$ ) registered for the plots of all the LMBP ANN predicted results against their corresponding experimental results. Having verified the reliability of the developed model, the simulated results can adequately supply the necessary information for developing new sets of MWNTs/quartz nanocomposites that falls within the range of those tested in the previous study (Tijjani *et al.*, 2018), thereby eliminating the time-consuming, expensive and destructive experimental investigation route.

## REFERENCES

- Al-Jabar, A. J. A., Al-Dujaili, M. A. A., and Al-Hydary, I. A. D. (2017). Prediction of the physical properties of barium titanates using an artificial neural network. *Applied Physics A*, 123 (4), 274.
- Günaydın, H. M., and Do an, S. Z. (2004). A neural network approach for early cost estimation of structural systems of buildings. *International Journal of Project Management*, 22 (7), 595-602.
- Hopfield, J. J. (1982). Neural networks and physical systems with emergent collective computational abilities. *Proceedings of the national academy of sciences*, 79 (8), 2554-2558.
- Jain, A. K., Mao, J., and Mohiuddin, K. M. (1996). Artificial neural networks: A tutorial. *Computer*, 29 (3), 31-44.
- Liu, B., and Liu, Y.-K. (2002). Expected value of fuzzy variable and fuzzy expected value models. *IEEE transactions on Fuzzy Systems*, 10 (4), 445-450.
- Nazari, A., and Riahi, S. (2011). Prediction split tensile strength and water permeability of high strength concrete containing  $TiO_2$  nanoparticles by artificial neural network and genetic programming. *Composites Part B: Engineering*, 42 (3), 473-488.
- Nazari, A., and Riahi, S. (2013). Artificial neural networks to prediction total specific pore volume of geopolymers produced from waste ashes. *Neural Computing and Applications*, 22 (3-4), 719-729.
- Nwobi-Okoye, C. C., and Ochieze, B. Q. (2018). Age hardening process modeling and optimization of aluminum alloy A356/Cow horn particulate composite for brake drum application using RSM, ANN and simulated annealing. *Defence Technology*
- Rumelhart, D. E., Hinton, G. E., and Williams, R. J. (1986). Learning representations by back-propagating errors. *Nature*, 323 (6088), 533.
- Shabani, M., Mazahery, A., Rahimipour, M., Tofigh, A., and Razavi, M. (2012a). The most accurate ANN learning algorithm for FEM prediction of mechanical performance of alloy A356. *Kov. Mater*, 50, 25-31.
- Shabani, M. O., Mazahery, A., Rahimipour, M. R., and Razavi, M. (2012b). FEM and ANN investigation of A356 composites reinforced with B4C particulates. *Journal of King Saud University-Engineering Sciences*, 24 (2), 107-113.



- TIJJANI, Y., YASIN, F. M., ISMAIL, M. H. S., and ARIFF, A. H. M. (2018). Manufacturing and mechanical characterization of multiwalled carbon nanotubes/quartz nanocomposite. *Journal of the Ceramic Society of Japan*, 126 (12), 984-991.
- Tuntas, R., and Dikici, B. (2016). An investigation on the aging responses and corrosion behaviour of A356/SiC composites by neural network: The effect of cold working ratio. *Journal of Composite Materials*, 50 (17), 2323-2335.
- Varol, T., Canakci, A., and Ozsahin, S. (2018). Prediction of effect of reinforcement content, flake size and flake time on the density and hardness of flake AA2024-SiC nanocomposites using neural networks. *Journal of Alloys and Compounds*, 739, 1005-1014.
- Wilamowski, B. M., and Yu, H. (2010). Improved computation for Levenberg–Marquardt training. *IEEE transactions on neural networks*, 21 (6), 930-937.